

Mathematical Modeling and Analysis

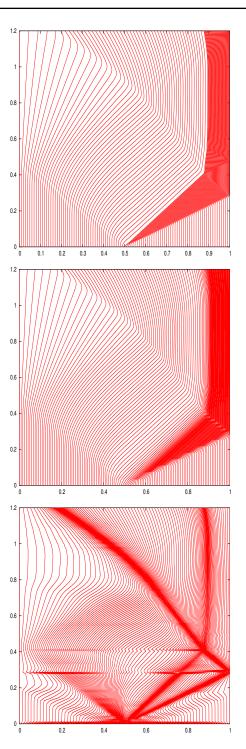
The Arbitrary-Lagrangian-Eulerian Code for 1D Compressible Flows

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The philosophy of the Arbitrary Lagrangian-Eulerian (ALE) methodology for solving multidimensional fluid flow problems is to move the computational grid, using the flow as a guide, to improve the robustness, accuracy and efficiency of a simulation. The main components in the ALE simulation are an explicit Lagrangian phase, a rezone phase in which a new grid is defined, and a remapping (conservative interpolation) phase in which a Lagrangian solution is transferred to the new grid.

In most ALE codes, the goal of the rezone phase is to maintain geometric quality of the mesh. The example of such a rezone strategy is the Reference Jacobian Matrix method [1]. It is intuitively clear that we may improve accuracy of the ALE simulation even more if the rezoned mesh has high geometric quality and at the same time minimizes some measure of a solution error. In the project, we have developed and implemented a Error-Minimization-Based rezone method [2]. The next figure shows trajectories of mesh points for the Sod shock tube problem. The accuracy of the pure Lagrangian simulation degrades quickly after time moment 0.4 due to bad representation of the shock wave. The RJM rezone strategy is not efficient in unpacking mesh points. The EMB rezone strategy captures all waves and results in much more accurate solution at time moment t = 1.2.

The goal of the remapping phase is to interpolate the physical fluid variables from the mesh obtained after the Lagrangian step to the rezoned mesh [3], [4]. This interpolation must (i) conserve the mass, momentum and total energy of the fluid, (ii) preserve positivity of density and specific internal energy, (iii) satisfy the maximum principle (no new extrema is created), and (iv) be



Trajectories of mesh points (vertical axis represents time) for the Sod shock tube problem: pure Lagrangian simulation (top); ALE simulation with the RJM rezone strategy (middle); ALE simulation with EMB rezone strategy (bottom).

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reversible. The last property states that if the new mesh coincides with the old one then the physical variables should not be changed by the remapping process. In the project, we have developed several repair methods ([5]). These methods are designed to enforce bounds for primitive variables by redistributing conservative variables (for example, density and mass). The bounds can be either physical (*i.e.*, the density must be positive and the concentration must be positive and less than one) or numerical (local maximum principle).

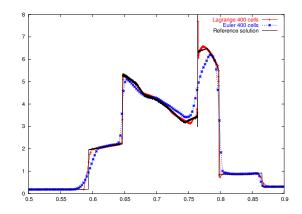
The Rezone and Remapping (R&R) components are implemented as C++ classes and can be easy incorporated into existing ALE codes. The presented figures have been obtained using the R&R components and the third component, the Lagrangian scheme. This numerical scheme is based on a compatible discretization [7] and explicit time integration of a system of 1D gas dynamics equations. The next figure shows density profiles for the Collela-Woodward blastwave problem. The "natural adaptivity" of the Lagrangian mesh allows us to get more accurate representation of solution features.

The R&R components support the Cartesian, cylindrical and spherical coordinate systems. They have been implemented following the basic code quality requirements [6]. Each of the components can be independently tested. The implemented unit tests allow verification and validation of each essential block of the code. The code is well documented which makes each of the components reusable. The R&R components have been implemented to test new rezone and remapping methods and to compare them with existing methods. The components are available on the SourgeForge website of the Los Alamos National Laboratory.

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Collela-Woodward blastwave: density profile at t = 0.038 in the Lagrangian and Eulerian simulations on a 400 cell mesh vs a reference solution.

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